Simulation of Browian Particles in a channel

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We study the behavior of ions with Brownian motion in the stationary state along a channel and the influence of external applied potentials and shapes of the channel. Our goal is to implement a 1-dimensional model that captures these effects by means of an effective potential and a diffusion coefficient. The method could be used as a tool to reduce the calculation cost of modeling these systems, which otherwise should be modeled in three dimensions.

I. INTRODUCTION

Ionic channels are small structures situated along the cell membranes that allow the exchange of charged particles between its two sides. They are crucial in some physiological processes, such as muscular contraction, liberation of neurotransmitters and regulation of genetic expression, among others.

We perform simulations of an open channel, so particles can freely enter or leave from both sides of the membrane. We consider that the concentration of ions outside of the channel remains constant despite the flux of ions. The membrane is modeled as a capacitor, with a voltage difference which does not depend on the flux of charges and remains constant.

Finally, we will consider that the particles do not interact with each other and move as Brownian particles, following the dynamics given by a Langevin equation. As the Reynolds number values associated to such small scales imply that the inertia is negligible, the problem can be formulated as a set of first order stochastic differential equations for the particle positions[1].

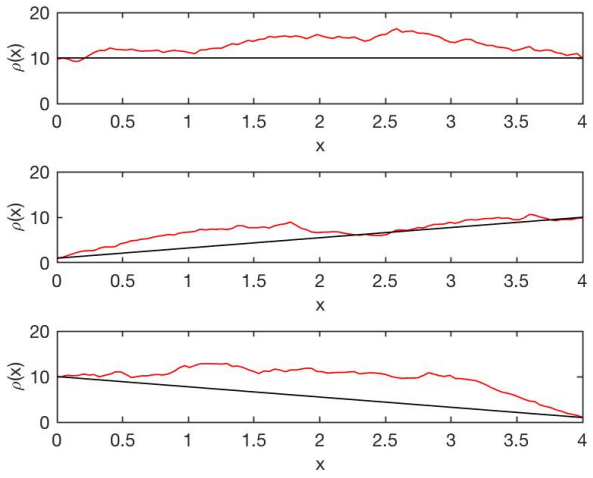

FIG. 1. Particle concentration vs position in steady state for different values of the boundary conditions ρ_1, ρ_2 in the case of null external potential. Top: $\rho_1 = \rho_2 = 10$; middle: $\rho_1 = 1, \rho_2 = 10$; bottom: $\rho_1 = 10, \rho_2 = 1$.

II. 1-DIMENSIONAL MODEL

We consider here the one dimensional dynamics in the x direction of the particles. Following the analysis done in [1], we have modeled the dynamics of the particles with a Langevin equation.

$$\gamma \dot{x} = -\frac{dV(x)}{dx} + \xi(t)$$

Here γ is a friction coefficient and $\xi(t)$ is a Gaussian white noise with zero mean and correlation given by

$$\langle \xi(t), \xi(t') \rangle = 2\gamma k_B T \delta(t - t')$$

In order to implement numerically the evolution of the particles, a temporal step Δt is considered and an explicit Euler algorithm is used to calculate the new position of a particle at time $t + \Delta t$ of the form:

$$x(t + \Delta t) = x(t) + f[x(t)]\Delta t + \sqrt{2D\Delta t}\chi$$

with $f(x) = -\frac{1}{\gamma}\frac{dV(x)}{dx}$, $D = \frac{k_B T}{\gamma}$ and χ a gaussian random number with zero mean and unit variance.

Finally, in order to perform our simulations, boundary conditions have been also implemented following the model developed in [1].

All simulations have been done using Matlab code and averaging on a single realization over a fixed temporal window in the steady state. The numerical values of the parameters chosen are: length of the channel $L = 4$, thermal energy $k_B T = 25$, friction coefficient $\gamma = 1000$ and temporal step $\Delta t = 10^{-4}$.

We begin considering the simplest case in which any force is applied to the channel. The results are shown in FIG. 1, where the black line represents the exact 1-D theoretical solution given by the Fokker-Planck equation for the concentration $\rho(x, t)$. In FIG. 1(top) the values of the concentration on both sides are the same and fixed to the value $\rho_1 = \rho_2 = 10$. As expected, the concentration in steady state is almost constant along the channel, with the value fixed by the boundary conditions.

We have also checked the symmetry of the problem applying, as shown shown in FIG. 1 (middle and bottom), different fixed values of the concentration in each side of the channel. As expected for this particular case, in

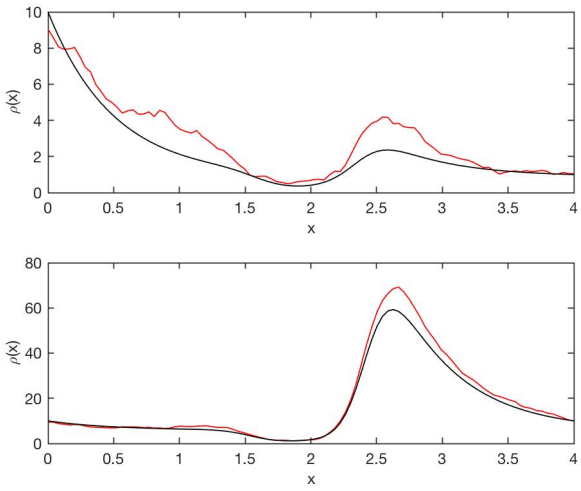

FIG. 2. Particle concentration vs position in steady state in the case where there is a constant external field, in addition to a potential barrier. Boundary conditions are fixed to the values: Top: $\rho_1 = 10, \rho_2 = 1.$; bottom: $\rho_1 = 10, \rho_2 = 10$.

the absence of a potential barrier, the final steady state concentration is close to a straight line connecting the fixed values at the boundary.

We have also considered the case where a constant external field is applied in addition to a potential barrier in the middle of the channel using the approach in [1]. The result is shown in FIG. 2 where the black line is the exact theoretical solution given by the Fokker-Plank equation in one dimension. In this case, the constant force term pushes the particles towards the left side, but they are trapped due to the barrier, and so the resulting flow is reduced.

It is interesting to compare both simulations , for instance FIG. 2 (bottom) and FIG. 1 (top), where boundary conditions are the same, but we do not have a potential barrier in the last case. Notice that in this last case no external constant force is considered, but under an external constant field the steady state concentration is in fact the same. In consequence, we can compare both simulation and understand what is the effect of the potential barrier. The straight line of the steady state solutions from FIG. 1 (top) disappears and the potential barrier induces an increase of the particle concentration at the side where the particles arrive due to the constant external applied field.

III. 3-DIMENSIONAL MODEL

In our simulations, we had modeled a cylindrical channel with variable radius depending on the longitudinal coordinate x. The dynamics of the particles are given by a Langevin equation, where the longitudinal coordinate behaves exactly as before, and the other coordinates are considered in diffusion. That is, the external force acting on the particles is exclusively in the x direction. We consider that the boundary conditions behave as the 1-D model, neglecting the fact that the number of entering particles depends on the surface of the channel, since all the results are proportional to it.

If a particle leaves the channel through a lateral wall and not through any of the open boundaries, we simulate the bouncing of the particle supposing a rectilinear trajectory between the current and previous position. We assume that the bouncing against the wall of the channel is like the bouncing against a plane wall tangent to the surface of the channel in the impact point. We first calculate the point of collision with a nonlinear equation solver and make a symmetrical reflection of the rest of the trajectory with this plane wall. To do so, we have parametrized the surface in cylindrical coordinates $surface(x, \theta) = [r(x), \theta, x]$ with two tangential vectors $[r'(x), 0, 1]$ and $[0, 1, 0]$, so the normal vector to the surface is the vectorial product of them, $normal = [-1, 0, r'(x)]$, that written in Cartesian coordinates is $normal = [r'(x), -y/r(x), -z/r(x)]$. From this, we calculate the new position of the particle reflecting the remaining part of the trajectory with respect to the defined plane. If the time step is small enough, the probability that the particle goes out from another lateral wall in the same time step is negligible, so we can implement a quite simple algorithm. Otherwise we would have to perform a loop in the number of collisions of each particle.

For the entering particles through the boundaries, we calculate the x coordinate as in the 1-dimensional case, but we have to determine the y and z coordinates in such a way that the particle falls into the channel boundaries. In cylindrical coordinates we choose the radius and the angle of the position of the entering particle. The angle can be easily obtained with a uniform probability density in $(0, 2\pi)$, multiplying 2π by a uniform random number in $(0, 1)$. However, the generation of the radius has to take into account that the probability density function must satisfy: $f(r) \propto 2\pi r$. Thus, we define the distribution function:

$$F(r) = C \int_0^r r = \frac{C}{2} r^2 = \frac{r^2}{r(x)^2}$$

We have applied the normalization condition that $F(r(x)) = 1$. Then, we can obtain a radius by generating a uniform random number $\chi \in (0, 1)$ and inverting the distribution function:

$$F(r) = \chi \Rightarrow r = F^{-1}(\chi) = r(x) \cdot \sqrt{\chi}$$

This is a very powerful method that allow us to generate random numbers of any distribution given by $F(r)$[2].

We have chosen a radius $r(x) = 1-(1-r_{\min}) \exp(-(x-2)^2)$, so it is smooth enough to perform well in later 1-D

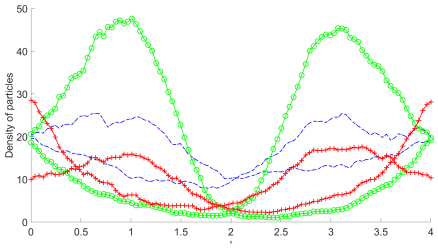

FIG. 3. Particle density vs position x in stationary state with positive and negative force of $|f| = 8k_BT/(\gamma L)$. Blue(- -) curve with a minimum radius of 0.5. Green(-o-) curve with a minimum radius of 0.1. Both curve with the same particle density at both boundaries of 20. The red(-+-) curve with a minimum radius of 0.25, with different boundary conditions at each side, one with density 10 and the other with density 30, and force heading from the low density into the high density.

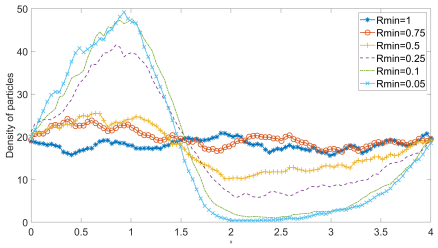

FIG. 4. Particle density vs position in stationary state for a positive force $f = 8k_BT/(\gamma L)$, equal density at both boundaries of value 20 and different sizes of the minimum radius.

effective models. The position of the minimum radius is located at the middle of the channel ($x = 2$), and the minimum radius is a depends on the simulation we perform.

The force is a few orders of magnitude around the value of $k_BT/(\gamma L)$ because, otherwise, the force would be so big that the random perturbations of the Brownian movement would not have any effect, or so small that the force would not be noticeable, compared to the diffusive term, so the movement of each particle would be a random unbiased path.

In FIG. 3, we can observe that the boundary conditions are satisfactorily fulfilled, since the density of particles in the extremes of the channel in stationary state remains close to the density of particles outside in all cases. The solution is symmetric with respect to the force and boundary conditions, which means that an opposite force and exchanging the densities of the source leads to a symmetric solution.

The value of the minimum radius has a big impact in the profile of the density of particles. On one hand, a big radius is not noticed by the particles. On the other hand, if the constraint is too small, it is difficult for the particles to cross the constraint, and they tend to accumulate before it. After the narrowing, there is a smaller density of particles, as the average time that particles

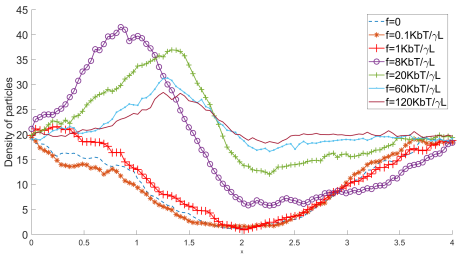

FIG. 5. Particle density vs position x in stationary state with positive force $f = 8k_BT/(\gamma L)$, minimum radius of 0.25 and different magnitudes of the dragging force.

remain in this region is small because of the action of the force. In FIG. 4, we can see that the smaller the minimum radius gets, the higher is the maximum before and lower is the minimum after the constraint, because it takes longer for the particles to go through the hole. Surprisingly, the change in the profile is quite abrupt when we change from a value of the minimum radius of $r_{\min} = 0.25$ to $r_{\min} = 0.5$, making that the steady state solution for $r_{\min} \geq 0.5$ is almost a constant; that is, the system does not see the narrowing in steady state.

We can also study how different magnitudes of the force affect the particle density in the stationary state. In FIG. 5 we see that, for forces smaller than $1k_bT/(\gamma L)$, the difference with a random movement ($f = 0$) is almost negligible, and the densities are proportional to the square of the radius, since the movement is driven by the diffusion motion. For intermediate forces, there is an accumulation before the constraint, as the particles tend to go to the right and bounce back until they find the way out to the other side of the narrowing. As the force grows, the particles tend to go to the right with more probability, so they find the way out faster. This provokes a smaller accumulation of particles before the narrowing, and a bigger density after it. In the high forces limit, the presence of the constrain is less relevant, and the system behaves in a similar way to a cylindrical channel without any narrowing.

IV. 1-DIMENSIONAL EFFECTIVE MODEL: THE FICK-JACOBS EQUATION

Our goal in this section is to derive an effective simulation in one dimension which reproduces the behavior of the system in three dimensions, specially when the channel presents a narrowing. In order to do so, we want to simulate the system with an equation similar to a Langevin equation, but the equation from section II is not enough because it does not take into consideration the narrowing of the channel. A priori one may think that it would be enough to add a potential barrier proportional to the narrowing of the channel, but a more detailed analysis shows us that this is not the

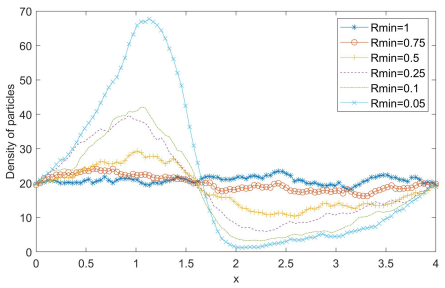

FIG. 6. Stationary state for different values of the minimum radius of the channel, under the same conditions as FIG. 4

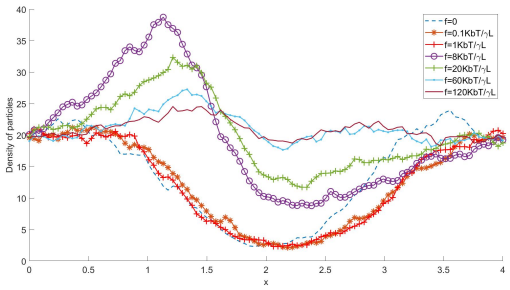

FIG. 7. Stationary state for different values of the drift force, under the same conditions as FIG. 5

case. The correct implementation, the validity of which depends on how abrupt is the narrowing of the channel, is derived from the Fick-Jacobs equation. We can rewrite this equation as an effective Fokker-Planck equation in 1 dimension [3–5].

We start from this effective Fokker-Planck equation in 1 dimension:

$$\frac{\partial P(x,t)}{\partial t} = -\frac{\partial}{\partial x}h(x)P(x,t) + \frac{\partial^2}{\partial x^2}D(x)P(x,t)$$

We assume that the diffusion depends on the position, as well, and that this dependence is of the form: $D(x) = D_0 \cdot g(x)$, where $g(x)^2 = \frac{1}{\sqrt{1+w'(x)^2}}$, and $w(x) = L\sqrt{\frac{S(x)}{\pi}}$ is the effective radius of the channel. After some manipulation we get to the following result:

$$\gamma\dot{x} = -2g(x)g'(x)kT + g(x)^2(F(x) + kT\frac{d\ln(S(x))}{dx}) + g(x)\xi(t)$$

$\xi(t)$ is a random number with the same autocorrelation as in the simple 1-dimensional model (section I). This equation resembles a Langevin equation, but we get some extra terms, depending on g, which we will have to implement in order to get the same results as for the 3d case. We have done simulations with the same parameters as in the previous section. The results can be seen in FIG. 6, 7 and 8.

In FIG. 6 we see that, for a radius greater or equal to R=0.1, the results are quite similar to the 3d case, although for R=0.05 the peak which appears before x=2

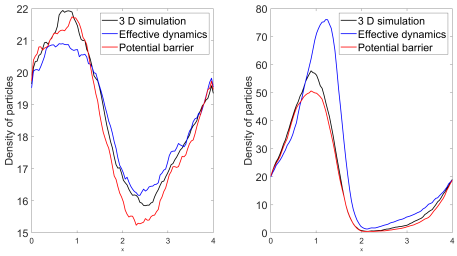

FIG. 8. Comparison of the stationary state for different models. We have taken $\rho_1 = \rho_2 = 20, f = 8k_BT/(\gamma L)$, int he left we have $r_{min} = 0.8$ and in the right $r_{min} = 0.05$

is quite larger. This is consistent with the fact that the approximation we have used is only valid for not very abrupt changes in the radius of the channel. In FIG. 7 we can observe similar results as in FIG. 5, as well. In order to get a more precise idea of the accuracy of this model with respect to the 3d model, we have performed three simulations, using in first place the 3-dimensional model, in second place the effective 1-dimensional dynamics derived from Fick-Jacobs equation, and in third place the dynamics in 1-dimension by just adding a potential barrier, proportional to the narrowing of the channel. The results are shown in FIG. 8. We see that this method does not behave properly for very abrupt narrowings, and even the simple 1-dimensional model with a potential barrier works better. However, for intermediate radii, the effective dynamics seem to work better for low densities but worse for big densities. In any case, the fluctuations in the solution make it hard to extract any reliable conclusion.

V. CONCLUSIONS

We have simulated the transport of ion through an ionic channel using different models. When modeling these problem we must take into account the three dimensions of the system. If we model these dynamics using a Langevin equation we obtain the expected results, in terms of the behavior of the system when a narrowing of the channel is present or when an external electric field is applied.

However, we can simplify the problem to a 1-dimensional case via the Fick-Jacobs equation, which reproduces the existence of narrowings in the channel. This model requires some approximations which, as we have seen from our simulations, become imprecise when the narrowing is very abrupt (FIG. 8). For intermediate radius, the effective dynamics no reliable conclusions can be extracted from our simulations. A much more accurate simulation should be carried out in order to determine the validity of the model, with probably much more iterations than the 60 million we have carried out.

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